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近年、３次元透過型電子顕微鏡の出現により、３次元で相分離構造の測定が行うことができるようになってきた。この実験で得られた構造を上で自己無撞着場計算を行うことで、実験で得られた構造に対して、更に詳細な鎖の情報の抽出が行える事が分かってきた。本発表では、その手法の概要と、対称ブロックポリマーによるラメラ構造に対して本方法を適用し、鎖の伸び等に関して解析を行ったので報告する。

1 Introduction

Three dimansional observation of the bulk stricture in polymer material is one of the hottest topics in the polymer science. Recently, Jinnai and co-workers have reported many results of the 3d observation studies using three dimensional transmissin electon microscopy (TEM). Using the 3d TEM, the phase separated structures can be obtained, and its resolution is about 1nm scale. This length scale can be applicable to the observations of the micro-phase separated structure, however cannnot be to those of the chain structures.

On the other hand, using the self consistent field (SCF) simulation, although the area of the simulated region is small (about less than 100nm), the information of the chain structure, for example, the end segment distribution or junction distribution, can be obtained. In this study, we propose a combinatorial method between the 3d TEM imaging and the SCF simulations on the three dimensional platform.

2 Method

To combine the 3d TEM imaging and the SCF simulations, the 3d structure obtained by experiments must be converted to the initial structure for the SCF simulation. We add the imaging interface to the platform of the OCTA, which we call as "Gourmet." Using this interface, we

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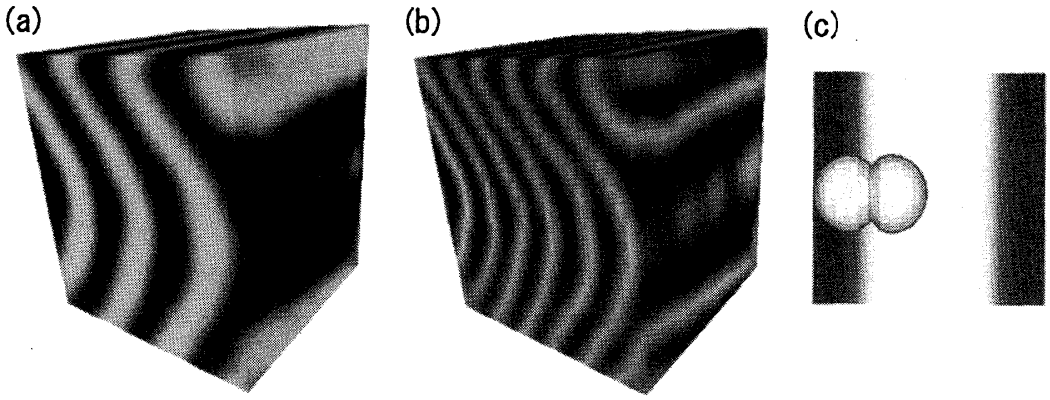

Figure 1: Results of SCF simulations. (a), (b), and (c) show the density distributions for the total PS, the junctions, and one chain, respectively.

make the converter program from the sliced image files to the volume fraction data. The original 3d TEM structures are observed by Jinnai et al, and the sample is the lamella structure of symmetric polystyrene-polyisoprene (PS-PI) block copolymer.

Using the converted structures, we perform the self consistent field simulation. In this simulation, the mean field potential, which is suitable for the given density profile, is estimated. Detail of the self consistent field method is refered in other papers.

3 Results

Figure 1 shows the density distribution of (a) total PS segment, (b) the junction segment, and (c) one chain which junction is grafted at PS-PI interface, respectively. Fig.1(b) and (c) is obtained by SCF simulation. The junctions are distributed at the interface of PS and PI. In one chain distribution, although the distribution of the horizontal direction to the lamella interface is not correctly calculated due to no randomness in this direction, the distribution to the vertical direction can be calculated. For example, $Rg_{vertical}$ calculated by one chain distribution is almost same as the values measured by Hasegawa et al in experiments. The result of the one chain distribution for the bent lamella will be shown in the presetation.

References

[1] H. Jinnai, T. Ikehara, T. Nishi, Adv. in Polym. Sci. **170** (2004) 115.

[2] E. Helfand, Z. R. Wasserman, Macromolecules, **9** (1976) 879; M. W. Matsen, M. Schick, Phys. Rev. Lett., **72** (1994) 2660.

[3] H. Hasegawa, T. Hashimoto, H. Kawai, T. P. Lodge, E. J. Amis, C. J. Glinka, C. C. Han, Macromolecules, **18** (1985) 67.